

## WHAT IS CLAIMED IS:

1. A method of conducting a mixture experiment, comprising:

determining an experimental space comprising n factors and a first factor in M number of factor level intervals and in a range of  $A_{\min}$  to  $A_{\max}$  where A is a proportion of the factor level to total factor levels; and

conducting an experiment on the first factor sampled in a range of levels determined according to a relationship  $(A_{\min} + (A_{\max} - A_{\min})/(n(M-1)))$  to  $(A_{\max} - (A_{\max} - A_{\min})/(n(M-1)))$ .

2. The method of claim 1, where the experimental space comprises a first factor in 0 to 100 levels and the first factor is sampled in a range of levels determined according to a relationship  $(100/(n(M-1)))$  to  $(100-200/(n(M-1)))$ .

3. The method of claim 1, wherein the factors are components of a catalyst.

4. The method of claim 1, wherein the space comprises the first factor in increments of  $1/(M-1)$  within the range.

5. The method of claim 1, wherein the experimental space comprises a three component mixture and a second factor level range is determined from a minimum level value to a maximum level value according to the relationship  $(100/(3(M'-1)))$  to  $(100-200/(3(M'-1)))$ , where  $M'$  is a number of level intervals for the second component.

6. The method of claim 1, wherein the experimental space comprises a three component mixture and a second factor level range is determined from a new minimum level value to a new maximum level value according to the relationship  $(100/(3(M'-1)))$  to  $(100-200/(3(M'-1)))$ , where  $M'$  is a number of level intervals for the second component and the space comprises the first factor in increments of  $1/(M-1)$  within its range and the second factor in increments of  $1/(M'-1)$  within its range.

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7. The method of claim 1, wherein the experimental space comprises a three component mixture and a second factor level range is determined from a new minimum level value to a new maximum level value according to the relationship  $(100/(3(M'-1)))$  to  $(100-200/(3(M'-1)))$ , where  $M'$  is a number of level intervals for the second component and the space comprises the first factor in increments of  $1/(M'-1)$  within its range and the second factor in increments of  $1/(M'-1)$  within its range;

and the method further comprises:

determining values for levels of a third factor of the mixture from a positive difference between 1.0 and values for a summation of levels of the other factor levels; and

conducting an experiment on samples defined according to the determined values for each factor.

8. The method of claim 1, wherein the experimental space comprises a four component mixture and a second factor level range is determined from a new minimum level value to a new maximum level value according to a relationship,  $(100/(3(M'-1)))$  to  $(100-200/(3(M'-1)))$ , where  $M'$  is a number of level intervals for the second component.

9. The method of claim 1, wherein the experiment comprises a CHTS experiment.

10. The method of claim 9, wherein the experiment is a CHTS experiment comprising steps of:

preparing a combinatorial library comprising a plurality of reagent compositions according to the experimental space;

effecting parallel reaction of the library to produce products; and

evaluating the products to select a lead from the library of reactants.

11. The method of claim 9, wherein the CHTS experiment comprises providing a reactor plate comprising a substrate with an array of reaction cells containing at least one reactant according to the experimental spaces and reacting the reactant in parallel with other reactants.

12. The method of claim 9, wherein the CHTS comprises effecting parallel chemical reactions of an array of reactants defined according to the experimental space.

13. The method of claim 9, wherein the CHTS comprises effecting parallel chemical reactions on a micro scale on reactants defined according to the experimental spaces.

14. The method of claim 9, wherein the CHTS comprises an iteration of steps of simultaneously reacting a multiplicity of tagged reactants prepared according to the experimental space and identifying a multiplicity of tagged products of the reaction and evaluating the identified products after completion of a single or repeated iteration.

15. The method of claim 9, wherein the experimental space factors comprise reactants, catalysts and conditions and the CHTS comprises

(A) (a) reacting a reactant selected according to the experimental space under a selected set of catalysts or reaction conditions; and (b) evaluating a set of results of the reacting step; and

(B) reiterating step (A) wherein a selected experimental space selected for a step (a) is chosen as a result of an evaluating step (b) of a preceding iteration of step (A).

16. The method of claim 9, wherein the factors include a catalyst system comprising a Group VIII B metal.

17. The method of claim 9, wherein the factors include a catalyst system comprising palladium.

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18. The method of claim 9, wherein the factors include a catalyst system comprising a halide composition.

19. The method of claim 9, wherein the factors include an inorganic co-catalyst.

20. The method of claim 9, wherein the factors include a catalyst system includes a combination of inorganic co-catalysts.

21. The method of claim 9, wherein the factors comprise a reactant or catalyst at least partially embodied in a liquid and effecting the CHTS method comprises contacting the reactant or catalyst with an additional reactant at least partially embodied in a gas, wherein the liquid forms a film having a thickness sufficient to allow a reaction rate that is essentially independent of a mass transfer rate of additional reactant into the liquid to synthesize products that comprise the results.

22. The method of claim 1 wherein the experiment is a CHTS experiment that identifies at least one point comprising an improved result; and the method further

comprises: defining at least one additional experimental space comprising at least one lattice of points representing reaction factor levels in a smaller increment around the point of lead result;

conducting at least a next CHTS experiment on the experimental space to identify at least one point comprising a lead result comprising a set of levels of reaction factors.

23. A method for defining a reduced set of samples for an experimental space and conducting an experiment on the samples,

comprising:determining an experimental space comprising n factors in M number of evenly spaced factor level intervals over a range of  $A_{min}$  to  $A_{max}$  where A is a proportion of a factor level to total factor levels;

specifying new factor level ranges for each factor according to a relationship  $(A_{\min} + (A_{\max} - A_{\min})/(n(M-1)))$  to  $(A_{\max} - (A_{\max} - A_{\min})/(n(M-1)))$ ;

selecting samples of combinations of factors in a set of M-1 evenly spaced levels within the specified levels; and

conducting an experiment on the samples.

24. The method of claim 23, comprising selecting only possible combinations of evenly spaced factor levels within the specified ranges.

25. The method of claim 23, comprising selecting all possible combinations of evenly spaced factor levels within the specified ranges.

26. A system for conducting an experiment, comprising;

a reactor for effecting a CHTS method on an experimental space to produce results; and

a programmed controller for the reactor that defines an experimental space comprising a lattice of points representing increments of reaction factor levels from a minimum level value to a maximum level value according to the relationship  $(A_{\min} + (A_{\max} - A_{\min})/(n(M-1)))$  to  $(A_{\max} - (A_{\max} - A_{\min})/(n(M-1)))$  where M is a number of intervals for the factor levels of the range, n is a number of mixture components and A is a proportion of the factor level to total factor levels.

27. The system of claim 26, wherein the controller is a computer, processor or microprocessor.

28. The system of claim 26, further comprising a dispensing assembly to charge factor levels of reactants or catalysts representing the catalyzed chemical experimental space to wells of an array plate for charging to the reactor.

29. The system of claim 26, wherein the dispensing assembly is controlled by the controller to charge factor levels of reactants or catalysts according to the controller defined space.

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30. The system of claim 26, further comprising a detector to detect results of the CHTS method effected in the reactor.

31. A system for conducting an experiment, comprising;  
a reactor for effecting a CHTS method on an experimental space to produce results; and

a programmed controller for the reactor for inputting experimental space information comprising n factors in M number of factor level intervals and in a range of  $A_{\min}$  to  $A_{\max}$  where A is a proportion of a factor level to total factor levels, specifying new factor level ranges for each factor according to a relationship  $(A_{\min} + (A_{\max} - A_{\min})/(n(M-1)))$  to  $(A_{\max} - (A_{\max} - A_{\min})/(n(M-1)))$  and selecting samples of combinations of factors in a set of M-1 evenly spaced levels within the specified levels for charge to the reactor.

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